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Confined Self-Assembly of Block Copolymers¹

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Spontaneous formation of ordered structures from amphiphilic molecules has attracted tremendous attentions in the last decades. Among the many different amphiphilic systems, block copolymers with their rich phase behavior and ordering transitions have become a paradigm for the study of structural self-assembly. In a physically confined environment, structural frustration, confinement-induced entropy loss and surface interactions can strongly influence the molecular organization. In particular, it is possible that confinement can lead to unusual morphologies which are not accessible in the bulk, thus providing opportunities to engineer novel structures. For confined asymmetric diblock copolymers, a rich variety of novel morphologies, ranging from helices to toroids to complex networks, is expected. The complexity of the possible structures presents computational challenges in simulations of macromolecular assemblies under confinement. We have used a combination of simulated annealing method and self-consistent field theory to exam the self-assembly of block copolymers confined in different geometries. A generic structural evolution path is obtained for the confined systems. The study demonstrates that confined self-assembly of amphiphilic molecules provides a robust method to produce nanoscopic structures which are not accessible in the bulk phases.

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